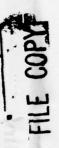


AeroChem TP-368



A COMPUTER CODE FOR FULLY COUPLED, TWO-PHASE ROCKET NOZZLE FLOWS



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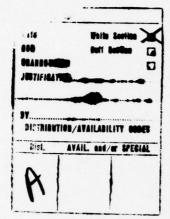
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These calculations describe the sensitivity of the unified code to variations in start line conditions, particle sizes, mass loading, and particle drag and heat transfer coefficients.



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I. INTRODUCTION

This report describes the development of a unified rocket nozzle computer program that is intended to serve as an aid in the study of the physical and chemical processes that control rocket exhaust plume dynamics, including plume visibility.

Low smoke propellants produce a small mass fraction of primary smoke particles at the nozzle exit; hence condensation in the plume is critical to the production of secondary smoke and thus plume visibility. Primary smoke particles, though, play an important role in plume visibility by serving as nucleation sites for secondary smoke, and therefore a complete determination of plume visibility requires, in addition to equilibrium condensation boundary considerations, an accurate description of nozzle exit plane particle properties.

To improve nozzle exit plane predictive capability, a new computer code has been developed by incorporating the two-phase transonic flow solution of Kliegel and Nickerson¹ (TSNIC) into the AeroChem FULLNOZ code.² This development allows the use of chamber initial conditions to generate a continuous nozzle calculation, thus eliminating the assumptions of supersonic start line gas and particle properties previously required by FULLNOZ.

The use of FULLNOZ in the supersonic regime offers powerful calculational capabilities by simultaneously treating gas/particle nonequilibrium, non-equilibrium chemistry, diffusion across streamtubes, and (optional) the turbulent boundary layer. The new code will enable the accurate determination of particle spatial distributions, velocity, and thermal lags at the nozzle exit plane and provide complete input information for subsequent plume calculations.

The following sections give a brief description of the techniques employed in TSNIC and FULLNOZ. A parametric study has been made to show the sensitivity of the solution to variations in (i) supersonic start line parameters due to transonic approximations, (ii) particle sizes and size distributions over a range

Kliegel, J.R. and Nickerson, G.R., Axisymmetric Two-Phase Perfect Gas Performance Program, TRW-02874-6006-R000, April 1967.

Pergament, H.S. and Thorpe, R.D., "A Computer Code for Fully-Coupled Rocket Nozzle Flows (FULLNOZ)," AeroChem TP-322, AFOSR-TR-75-1563, NTIS AD A019 538, April 1975.

applicable to low signature propellants, and (iii) particle drag and heat transfer coefficients over the applicable range. A complete description of program input, a sample input, and a sample output are given in Appendixes A, B, and C, respectively.

II. CODE DESCRIPTION

A. TSNIC

TSNIC is fully described in Ref. 1. A perturbation method is employed to attain an approximate solution to the subsonic and transonic governing equations of gas/particle equilibrium flow. The solution includes velocity and thermal lags between gaseous and inert condensed phases. One dimensional sink flow is assumed in the converging section of the nozzle, and gas/particle properties are determined on the sink line. The transonic region is divided into several zones and perfect gas assumptions are used to obtain gas properties. Particle trajectories are calculated through the throat region to determine particle properties on the supersonic start line. The gas/particle expansion, including nonequilibrium effects is approximated in each zone with an average expansion coefficient (see Fig. 1).

TSNIC uses as input chamber properties (such as produced by standard equilibrium codes), particle sizes, distributions and mass loading, and throat geometry parameters. Values of the gasdynamic state and particle velocity and thermal lags are interpolated on the start line for a specified number of points.

B. FULLNOZ

The FULLNOZ code is fully described in Ref. 2. It is based on the MULTITUBE method of Boynton³ which uses the streamtube method to integrate the hyperbolic governing equations of supersonic flow. In this method, the elliptic Navier-Stokes equations are reduced to hyperbolic form by assuming that diffusional effects along streamlines are small compared to diffusion across streamlines. This assumption is very good for rocket nozzle flows and enables one to solve an initial value problem (where a marching procedure can be used)

^{3.} Boynton, F.P., "The MULTITUBE Supersonic Flow Computer Code," General Dynamics/Convair GDC-DBB 67-003, February 1967.

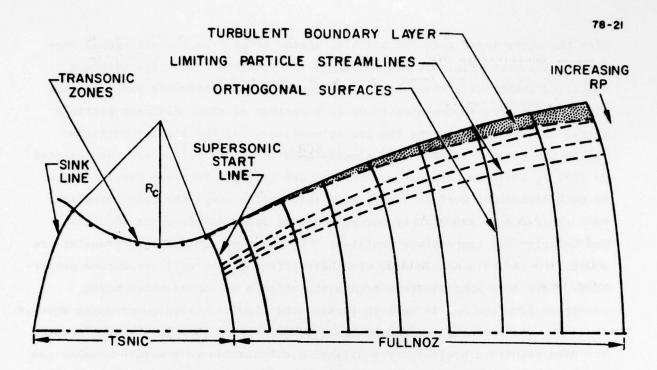


FIGURE 1 TSNIC/FULLNOZ SCHEMATIC

rather than the more difficult boundary value problem. The gas flow equations, in finite-difference form, are solved along and perpendicular to streamlines while a full continuum particle cloud system of equations is incorporated for the condensed phase.

The advantages of using the streamtube method over the method-of-characteristics in calculating rocket nozzle flows are: (i) species diffusion, shear, and heat transfer normal to streamlines are easily included; (ii) chemical reactions or internal relaxations are easily incorporated since the calculation follows streamlines; (iii) bounding surfaces and gradients normal to streamlines are treated without difficulty; and (iv) a wide variety of boundary conditions including mass transfer, shear, and heat transfer can readily be incorporated.

FULLNOZ utilizes the following information: (1) initial gas and particle properties in the supersonic region just downstream of the nozzle throat (supplied by TSNIC), (2) the nozzle wall contour, (3) a chemical reaction mechanism and rate coefficients, (4) physical properties of the particles, and (5) the nozzle wall temperature (for the boundary layer calculations).

With the above input data the marching scheme steps from one orthogonal surface to the next (Fig. 1), computing gas and particle properties within a specified number of streamtubes. The (essentially) continuous particle size distributions are represented by up to a maximum of eight discreet particle sizes. All particles cross the gas streamlines, but the lighter particles follow the gas streamlines more closely than the heavy particles. As depicted in Fig. 1, limiting particle streamlines are computed for each particle size. At each orthogonal surface (i.e., each integration step) the code calculates wall shear stress and heat transfer, boundary layer displacement thickness, and velocity and temperature profiles. The shear stress and heat transfer are coupled to the main nozzle flow via their effect on the wall streamtube properties. This code approximately treats the effects of shocks which might originate from the nozzle wall in turning the flow as strong compression waves.*

The operation of the combined TSNIC/FULLNOZ code is straightforward, but does require a preliminary equilibrium calculation to generate chamber gas properties. Because TSNIC does not treat chemical kinetics, chemical equilibrium (or interpolation between equilibrium and frozen flow) can be assumed to extend to the throat region to obtain the composition data used by FULLNOZ. This procedure provides acceptable accuracy in many situations and equilibrium codes such as the RPL-ISP program⁵ are especially suitable for providing such information. If greater accuracy is required, a separate kinetic calculation can be made between the chamber and throat using a code such as the AeroChem nonequilibrium streamline code (NEQSLINE). A complete description of program input is given in Appendix A.

^{*} Nozzle shocks could be incorporated into FULLNOZ in a manner similar to that employed in the AIPP Code to detect internal plume shocks, but this would require additional programming.

^{4.} Pergament, H.S. and Kelly, J.T., "A Fully-Coupled Underexpanded Afterburnning Rocket Plume Program (The AIPP Code). Part II. Program User's Manual," Final Report, AeroChem TP-328, AFRPL-TR-75-52, NTIS AD A019 411, December 1975.

^{5.} Selph, C. and Hall, R., "Theoretical ISP Program," AFRPL, Edwards, CA, 1974.

^{6.} Pergament, H.S. and Mikatarian, R.R., "Prediction of Minuteman Exhaust Plume Electrical Properties," AeroChem TP-281, May 1973.

III. CODE TESTING

In order to determine performance characteristics for the TSNIC/
FULLNOZ code, a parametric set of calculations was made to test for the sensitivity of the solution to variations in: (i) start line properties, including those that result from assumptions concerning throat geometry and start line location, (ii) particle sizes and mass loading which were varied over a range expected in rocket nozzle flows, and (iii) particle drag and heat transfer coefficients, commensurate with the expected extremes in particle shapes.

The parametric calculations were made for a small motor using the N5 double base propellant. The 10.5° nozzle has a throat area of 0.72 cm² and an expansion ratio of 3.7. To save computation costs, and because the main interest is in the resultant particle properties at the nozzle exit, the comparisons were made with no kinetic or boundary layer calculations. The standard case employed the following values of key variables: (i) mass fraction of particles, WPWGT = 0.005; (ii) ratio of axial start line location to throat radius, ZAX = 0.7; (iii) particle radii, RP = 0.8, 1.25 μ ; (iv) drag and heat transfer coefficient factors, FFF and FFG = 1.0; (v) nozzle inlet angle, THID = 10.5°; and (vi) ratio of throat radius of curvature to throat radius, RRT = 3.0.

A. START LINE PARAMETERS

Key input specifications to the TSNIC code that affect supersonic start line computations are the throat geometry and the prescribed location of the start line. For many cases, the details of the throat geometry may not be known and estimated values must be input to the program. Hence, calculations were made varying the throat radius of curvature, $R_{\rm C}$, and the converging section inlet angle to test for their effect on start line and ultimately, exit plane gas and particle properties. It was found that changing the inlet angle from 10.5° to 15° produced nearly no change in start line or exit properties, indicating the solution is insensitive to this parameter. There is, however, a restriction in the selection of the $R_{\rm C}$, since smaller values increase the divergence of gas and particle streamlines at the throat, complicating the solution. Reference 7 recommends RRT = $R_{\rm C}/R^* > 1.5$ to allow the solution to

Coats, D.E., et al, "A Computer Program for the Prediction of Solid Propellant Rocket Motor Performance," AFRPL-TR-75-36, July 1975.

proceed but in the present use it was found that RRT greater than 2.0 was required. It is believed though, that this restriction does not alter the adequacy of the analysis for most cases of interest.

Another restriction in the use of TSNIC is in the prescription of the supersonic start line location. The axial location (downstream of the throat) can be estimated from the following source flow approximation:

ZAX =
$$\left\{ (RRT) \sin(THIW) + \frac{1 - \cos(THIW)}{\sin(THIW)} \right\}^{0.83}$$

where ZAX = $Z_{axis}/R*$ is the start line location and THIW is the nozzle wall angle. For the present case with THIW = 10.5° and RRT = 3.0, ZAX = 0.7. When ZAX was reduced to 0.5, TSNIC failed; when a value of 1.0 was used the resultant start line was geometrically inconsistent with the downstream nozzle geometry and the FULLNOZ calculation failed. Other considerations in the use of TSNIC are well documented in Ref. 7.

B. PARTICLE SIZES

Early studies⁸, of primary particle sizes in rocket motor exhausts indicated that the location of the distribution peaks depends on factors such as motor size and chamber pressure. For small motors size peaks in the 1 to 3 μ radius range were expected. More recent works¹⁰, indicate that the majority of particles are very small with radii less than 0.1 μ , although mass distribution peaks remain in the 1 to 3 μ range.

A series of calculations was planned to test the performance of the TSNIC/FULLNOZ program over this applicable range of particle sizes. Unfortunately, though, the assumptions employed in the TSNIC analysis result in

^{8.} Smith, P.W., Delaney, L.J., and Radke, H.H., "Summary Results of Particle Size Measurements," in <u>Proceedings of the AFRPL Two-Phase Flow Conference</u> 1967, AFRPL-TR-67-223, Vol. I., p. 264.

Rochelle, W.C., "Review of Thermal Radiation from Liquid and Solid Propellant Rocket Exhausts," NASA Marshall Space Flight Center, Huntsville, AL, NASA-TM-X-53579, February 1967.

^{10.} Dawborn, R. and Kinslow, M., "Studies of the Exhaust Products from Solid Propellant Rocket Motors," Arnold Air Force Station, Tullahoma, TN, AEDC-TR-76-49, September 1976.

^{11.} Varsi, G., "Summary of Particulate Measurements," NASA, Atmospheric Effects Working Group Meeting, Vandenberg AFB, October 27-28, 1976, p. 96.

serious computational difficulties when particles with radii less than 1 μ are encountered. Hence, the lower limit of the size range tested was limited to 0.8 μ . The upper limit of 2.5 μ was used as representative of the small motor.

Comparisons of gas and particle velocities and temperature are shown in Figs. 2 and 3 for particles of radii 0.8, 1.25 and 2.50 μ . A particle loading of 0.5% was used. Because of the low particle loading, the particles have a negligible effect on the gas properties and the profiles are uniform at the nozzle exit. The particles do not, however, completely follow the gas streamlines, as evident in Fig. 4. The angle ϕ is the flow angle of the particles relative to that of the gas. For most of the flow regime, the particle trajectories diverge more than that of the gas, except near the wall. The gas/particle divergence is, in all areas, quite small.

Increased effects of the gas/particle interaction are seen when particle loadings are increased to 30% (characteristic of highly aluminized propellants). Velocity and temperature profiles at the nozzle exit, shown in Figs. 5 and 6, indicate that the presence of particles does affect the exit plane gas properties. In these figures, case Al represents a calculation with particles of 0.8 and 1.25 μ radii, and case A2, 1.25 and 2.50 μ .

Other applications of the FULLNOZ code to variations in particle size are described in Ref. 12 for a large bell-shaped nozzle.

C. PARTICLE DRAG AND HEAT TRANSFER

The momentum and energy exchange between the spherical particle and gas flows is described completely in Ref. 2. In order to include nonspherical particles, alterations to the particle and heat transfer coefficients are necessary. Although liquid condensates would normally be spherical, solidification and agglomeration of certain species could form nonspherical particles. Dynamic shape factors, which relate the drag of an arbitrarily shaped particle to that of a sphere, are available in Ref. 13. For the extreme shapes of prolate and oblate ellipsoids, the increase in drag is within 50% of the spherical

^{12.} Thorpe, R.D., Pergament, H.S., and Hwang, B.C., "NO_X Deposition in the Stratosphere by the Space Shuttle Solid Rocket Motors," <u>JANNAF 9th Plume Technology Meeting</u>, CPIA Publ. 277 (Applied Physics Lab., Johns Hopkins Univ., Silver Spring, April 1976) pp. 317-352.

^{13.} Fuchs, N.A., The Mechanics of Aerosols (Pergamon Press, New York, 1964).

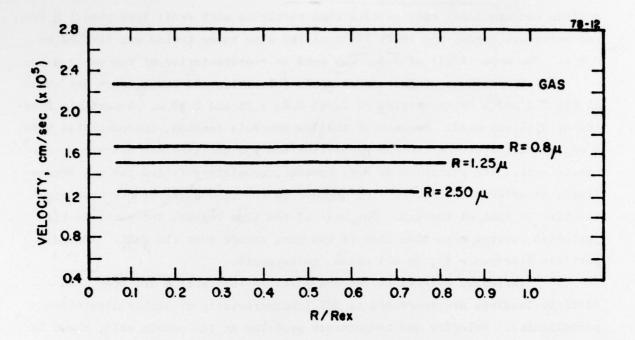


FIGURE 2 NOZZLE EXIT PLANE GAS AND PARTICLE VELOCITIES

Particle mass fraction = 0.5%.

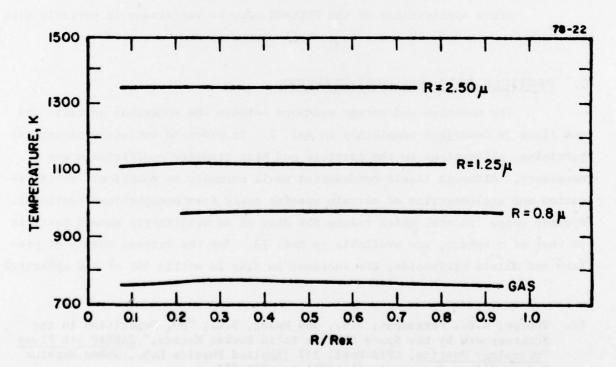


FIGURE 3 NOZZLE EXIT PLANE GAS AND PARTICLE TEMPERATURES

Particle mass fraction = 0.5%.

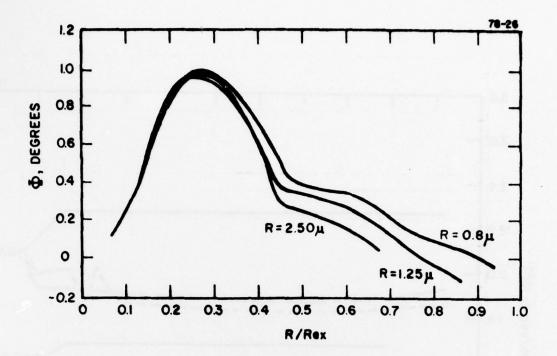


FIGURE 4 DIFFERENCE BETWEEN PARTICLE AND GAS TRAJECTORIES AT NOZZLE EXIT PLANE

drag. Since definitive information of the effect of particle shape on heat transfer was not available, these coefficients were assumed to be proportional to those for particle drag. The results of this calculation are shown in Figs. 7 and 8 for 1.25 μ particles. An increase in the drag to the upper limit yields a 10% decrease in both particle velocity and temperature. In order to more fully describe the sensitivity of the analysis and to account for uncertainties in particle data, the case of a decrease in these coefficients is also shown.

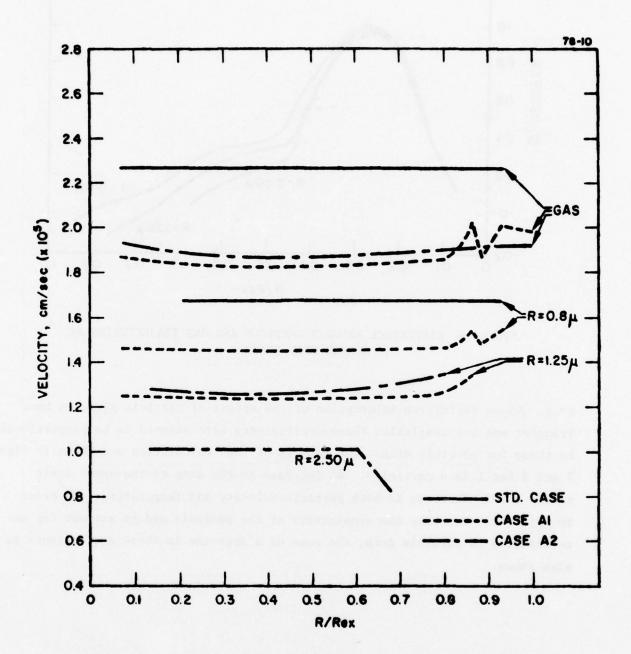


FIGURE 5 THE EFFECT OF PARTICLE MASS LOADING ON EXIT PLANE GAS AND PARTICLE VELOCITIES

Mass loading for standard case is 0.5%; for cases A1 and A2, 30%.

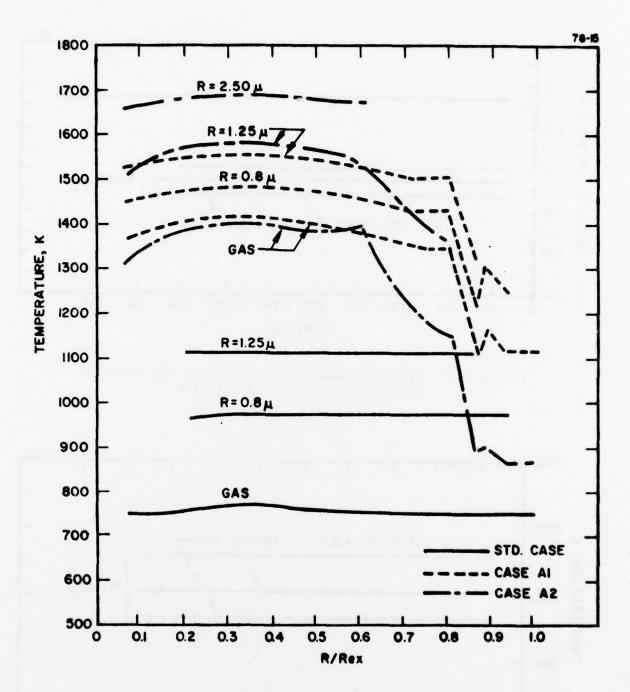


FIGURE 6 THE EFFECT OF PARTICLE MASS LOADING ON EXIT PLANE GAS AND PARTICLE TEMPERATURES

Mass loading for standard case is 0.5%; for cases Al and A2, 30%.

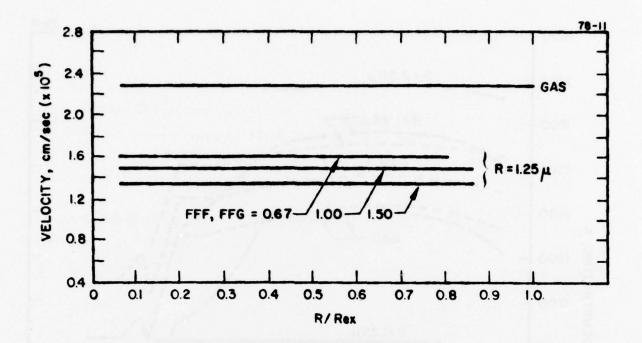


FIGURE 7 THE EFFECT OF VARIATIONS IN DRAG AND HEAT TRANSFER COEFFICIENTS ON PARTICLE VELOCITY

Particle mass loading = 0.5%.

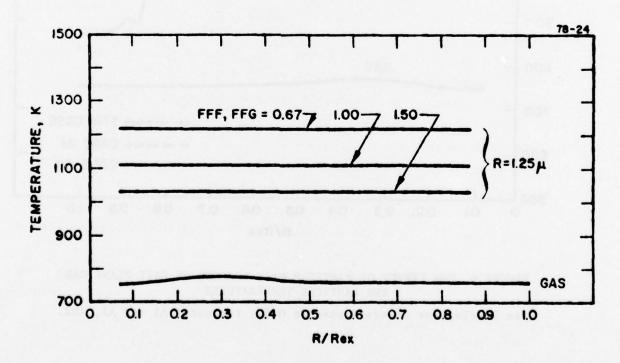


FIGURE 8 THE EFFECT OF VARIATIONS IN DRAG AND HEAT TRANSFER COEFFICIENTS ON PARTICLE TEMPERATURE

Particle mass loading = 0.5%.

IV. CONCLUSIONS

The incorporation of the Kliegel and Nickerson transonic, two-phase flow code into the AeroChem nozzle code has resulted in a powerful tool for the calculation of nozzle exit plane gas and particle properties. Although some care is required to properly specify throat geometrical parameters, and particle radii are limited to \$\geq 1.0 \mu\$, the code is applicable to a wide range of conditions. The calculated gas and particle properties at the nozzle exit for various particle sizes and mass loadings display expected behavior for conical nozzle flows. The major effect on particle concentrations at the exit is the size distribution; the effects of uncertainties in the particle/gas interaction, resulting from variations in particle shapes, is small.

V. RECOMMENDATIONS

The TSNIC/FULLNOZ code is an ideal basic tool for the study of fundamental processes that control the distribution of primary smoke particle concentrations at the nozzle exit. There is experimental evidence that primary smoke is strongly affected by chamber ballistic properties such as pressure, burn rate, mass flow, and propellant grain size. However, there are little or no primary smoke results described in terms of important nozzle processes such as high temperature condensation. A condensation model applicable to nozzle flows would treat the smallest particles as molecular groups which would diffuse with the gas. These groups would be treated as particles after attaining a predetermined size. An adequate treatment of this problem requires a transonic analysis with the capability of treating chemical kinetics and a wider range of particle sizes. Particle growth mechanisms such as coagulation might justifiably be ignored since the rates of these processes may be too slow to have a marked effect in the nozzle.

It is recommended then, that further efforts in describing primary smoke be directed toward the modeling of high temperature condensation, within the framework of a unified nozzle model such as the TSNIC/FULLNOZ code.

^{14.} Placzek, D.W., "Effect of Interior Ballistic Parameters on Rocket Exhaust Smoke," Rohm and Haas TR-S-282, November 1970.

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APPENDIX A

PROGRAM INPUT AND OPERATION

The TSNIC/FULLNOZ program was coded for CDC 6600 or 7600 computers. It is run in two job steps with separate input for TSNIC and FULLNOZ. Transfer of start line properties is made from TSNIC to FULLNOZ via scratch files: the gas properties on unit 2 and particle properties on unit 3.

I. TSNIC INPUT

All input to TSNIC is made through NAMELIST/DATA/. The input items are divided into three groups: (1) chamber products of combustion, (2) particle data, and (3) inlet and throat parameters. For some input items, values are assumed by the program and usually need not be supplied.

A. PROPELLANT DATA

Item	Input Quantity	Units
CAPN	viscosity temperature exponent, specific heat at constant pressure	none
GAMMA	specific heat ratio, C /C gp /C	none
GMGO	chamber gas viscosity coefficient	lbs/ft sec
PC	chamber pressure	psia
PR	Prandtl number	none
TGO	chamber temperature	°R
WMOLG	molecular weight of gas	none
B. PART	FICLE DATA	
CPL	particle heat capacity $(T_p > T_{p_m})$	cal/mole °K
CPS	particle heat capacity $(T_p < T_{p_m})$	cal/mole °K
D(J)	the diameter of each of n particles is to be input so that $D(1) < D(2) \dots < D(N)$ set $D(N+I) = 0$	microns

Item	Input Quantity	Units
HPI.	liquid particle enthalpy $(T_p = T_{p_m})$	kcal/mole
HPS	solid particle enthalpy $(T_p = T_{p_m})$	kcal/mole
ITOT	number of particle groups, N. $N \leq 8$ is required	none
SMP	particle density	lbs/ft3
TPM	particle solidification temperature	°R
WPWGT	ratio of particle to gas weight flow	none
WPWT(J)	particle weight flow fractions corresponding to each of the above particle diameters, D(J)	none

C. INLET AND THROAT PARAMETERS*

Item	Input Quantity	Units	Assumed Value
DZI	particle trajectory integration step size	none	0.002
DZMIN	inlet step size parameter	none	0.002
NILP	number of initial line points	none	15
RRT	ratio of throat radius of curvature to throat radius. A value $R_{\rm c} \gtrsim 2$ is required.	none	
RT	throat radius	ft	
THFD	faring angle (no faring for THFD $>$ THID)	degrees	5
THID	inlet angle	degrees	
THIW	intersection of initial line and wall	degrees	12.
THJD	angle defining the zone farthest downstream	degrees	9.
ZAX	ratio of intersection of initial line and axis to throat radius	none	
ZI	number of upstream zones	none	3
ZJ	number of downstream zones	none	2

^{*} See Fig. A-1

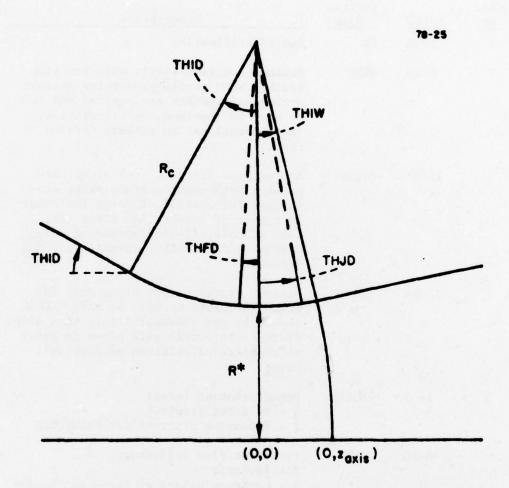


FIGURE A-1 INLET AND THROAT PARAMETERS

II. FULLNOZ INPUT

Input for the FULLNOZ portion of the program is given below.

Card No.	Cols.	Fortran Name	Description	Format
1	1-80	ID	Run identification	20A4
2	1-10	NSEC	Maximum run time (sec); when run time reaches NSEC nozzle properties at last orthogonal surface are punched and can be used to continue the calculation. (Not operational in present version of code.)	1.10
	11-22	DXLSS	Approximate distance (cm) along axis between orthogonal surface print stations. For control of print increment by number of integration steps (KP, Card 4, Cols. 11-15) instead of axial distance, make DXLSS larger than XLMAX (below).	E12.5
	23-34	XLMAX	Maximum distance (cm) along axis for which calculations will be made. XLMAX should be set somewhat larger than axial distance to nozzle exit plane in order to complete calculation at last wall point.	E12.5
3	1- 5	IBUGSH	Debug printout index; 0 - No debug printout 1 - Extensive printout for debugging	15
	6-10	ITURB	 Turbulent flow indicator; 0 - Inviscid 3 - Constant values of turbulent mixing parameters, μ, Pr and Le are input on Card 9. 	15
4	6-10	NN	Number of terms for C _p polynomial curve fit plus one; for curve fits supplied with program, NN = 6. If fewer coefficients are used for a given species NN is left at 6 and zeroes are input for the missing coefficients (see Card 7).	15
	11-15	КР	Output control; number of orthogonal surfaces between print stations. To control print via axial distance (DXLSS, Card 2, Cols. 11-22) instead of orthogonal surfaces set KP larger than LPLANE (Card 4, Cols. 36-40).	

Card No.	Cols.	Fortran Name	Description	Format
4	16-20	MMAX	Number of points needed to describe shape of inner boundary; always set equal to 2 for axis boundary.	15
	21-25	NMAX	Number of points required to define nozzle wall contour (50 maximum)	15
	26-30	NDS	Total number of gas species in flow (25 maximum)	15
	31-35	NITER	Maximum number of iterations allowed for iterative solutions (e.g., calculation of streamtube properties for variable γ) Recommended value: NITER = 50	15
	36-40	LPLANE	Maximum number of integration steps for entire calculation	15
	41-45	IKINE	Number of chemical reactions (40 maximum)	15
	NOTE:		DARY LAYER CALCULATIONS ARE TO BE MADE CARD 5	
5	1- 5	TWALL	Nozzle wall temperature (°K) (assumed constant)	F5.0
	8	IBLFLG	Boundary layer property printout indicator; 0 - Print Reynolds no., thickness and friction parameters 1 - Print above plus velocity and temperature profiles	11
	11	IBL	Boundary layer calculation indicator; 0 - No boundary layer calculation 1 - Calculate boundary layer	11
6	1- 9	АLРНАН	Factor that multiplies maximum stable step size; Recommended value: ALPHAH = 0.8	F9.4
	10-18	EPSLON	Amount by which streamtube Mach numbers must exceed one in order for the calculation to continue. Recommended value: EPSLON = 0.01	F9.4
	19-27	TOL	Convergence tolerance for iterative solutions; Recommended value: TOL = 1 x 10 ⁻⁴	F9.4

Card No.	Cols.	Fortran Name	Description Fo	ormat
6	28-36	DELTA	Metric exponent*; 0 - Two-dimensional flow 1 - Axially symmetric flow	9.4
	37-45	ATOL	Maximum allowable fractional change in streamtube area per step. Recommended value: ATOL = 0.1	9.4
	NOTE:		7 DEFINES THE THERMODYNAMIC DATA FOR EACH SPEC 2 CARDS PER SPECIES AND NDS SPECIES	CIES.
7.1.1	1-13	A(1)	L ₁ El	13.5
	14-26	A(2)	L ₂ Specific heat polynomial constants	
	27-39	A(3)	L ₃ for first species, (cal/mole °K)	
	40-52	A(4)	L ₄	
7.1.2	1-13	A(5)	L ₅ , Specific heat polynomial constant for first species	13.5
	14-26	A(6)	L ₆ , Enthalpy constant of integration Entrangement of first species	13.5
			$\left(\Delta H_{f}^{\circ} - \int_{0}^{298} C_{p} dT\right) \text{(kcal/mole)}$	
	27-39	CS(1)	L ₇ , Entropy constant of integration for first species (cal/mole °K)	
7.NDS.1 7.NDS.2			Repeat thermodynamic data for NDS species	
	NOTE:		8 IDENTIFIES EACH SPECIES AND SPECIFIES VARIOUP PROPERTIES. MUST BE IN SAME ORDER AS CARD GROUN	
8.1	1- 4	IDENT(1)	Species name; first species (the remain- ing data on Card 8.1 also apply to the first species)	4
	13-24	MUO(1)	Viscosity at reference temperature [†] EX (g/cm-sec); only used when flow contains particles. FOR NO PARTICLES, MUO MUST = 0 FOR ALL SPECIES	12.4

^{*} The particle conservation equations are written only for axially symmetric flow. Thus two-dimensional solutions can only be obtained for flows without particles.

[†] Values for common gases can be found in most physics and chemistry handbooks.

Card No.	Cols.	Fortran Name	Description	Format
8.1	25-36	TO(1)	Reference temperature for viscosity (°K)	E12.4
	37-48	OMEGA(1)	Exponent describing viscosity/temperature relation; $\mu \propto T^{\omega}$	E12.4
	49-60	PR(1)	Reciprocal of species Prandtl number	E12.4
	61-72	SC(1)	Reciprocal of species Schmidt number	E12.4
	73-80	MW(1)	Species molecular weight	E8.2
8.NDS			Repeat for each species	
	NOTE:	CARD 9 IS	NOT NEEDED IF ITURB = 0 (CARD 3 COLS. 6-10)	
9	1-10	TLE	Turbulent Lewis number (constant)	E10.3
	11-20 21 - 30	TPR EDDYK	Turbulent Prandtl number (constant) Eddy viscosity, g/cm-sec (constant)	E10.3 E10.3
10.1	1-10	C(1)	Mass fraction of first species	E10.3
	11-20	C(2)	Mass fraction of second species	E10.3
	71-80	C(8)	Mass fraction of eighth species	E10.3
10.2			Continue on subsequent cards; up to 25 species	8E10.3
	NOTE:		11 DEFINES THE NOZZLE WALL CONTOUR. FIRST (AT START LINE) IS TRANSFERRED FROM TSNIC.	
11.1	1-12	XB(2)	Axial position (cm) of second point along nozzle wall	E12.4
	13-24	RB(2)	Radial position (cm) of second point along nozzle wall	E12.4
11 (NMAX-	-1)1-12	XB(NMAX)	Final axial position of nozzle wall	E12.4
		RB (NMAX)	Final radial position of nozzle wall	E12.4
	NOTE:	CARDS 12 AND IN FLOW.	ND 13 ARE INCLUDED ONLY IF PARTICLES ARE	
12	1-10	FFF	Factor to adjust particle/gas drag coefficient	E10.3
	11-20	FFG	Factor to adjust particle/gas heat transfer coefficient	E10.3
	21-30	CL	Liquid particle specific heat (cal/g-°K)	E10.3

Card No.	Cols.	Fortran Name	Description	Format
12	31-40	CS	Solid particle specific heat (cal/g-°K)	E10.3
	41-50	HTRAN	Particle heat of solidification (cal/g)	E10.3
	51-60	WT	Particle molecular weight	E10.3
13	1-10	RHSS	Particle density (g/cm³)	E10.3
	31-40	TPS	Particle solidification temperature (°K)	E10.3
	NOTE:	RATE COEFF	ING CARDS CONTAIN THE REACTION MECHANISM AND TICIENTS. USE ONLY IF IKINE (CARD 4, COLS. GREATER THAN 0.	
14.1	1- 4	IZD(1)	Species A	A4
	7		+ sign	
	8-11	IZD(2)	Species B	A4
	14		+ sign	
	15-20		Blank or M	A4
	21		= sign	
	22-25	IZD(3)	Species C	A4
	28		+ sign (if needed)	
	29-32	IZD(4)	Species D	A4
	35		+ sign (if needed)	
	36-39	IZD(5)	Species E	A4
	49-50	IRR	Reaction type*	12
	51	IRT	Rate coefficient* type	11
	52-59	RC(1)	Pre-exponential factor, A (cm-molecule-sec units)	E8.2
	60-63	RC(2)	Temperature exponent, N	F4.1
L. Size	64-72	RC(3)	Activation energy, B (cal/mole)	F9.1
14.IKINE			Same as above for IKINE reaction	

^{*} See Appendix A, Section III for reaction and rate coefficient types. See Ref. 2 for a complete explanation of the reaction mechanism.

III. REACTION AND RATE COEFFICIENT TYPES

Ten possible reaction types are included in the program:

Reaction Type

(1)
$$A + B + M \neq C + D$$

(2)
$$A + B + M \neq C + M$$

$$(3) \qquad A + B \qquad \Rightarrow C + D + E$$

$$(4) \qquad A + B \qquad \neq C$$

$$(5) \qquad A + M \qquad \Rightarrow C + D + M$$

$$(6) \qquad A + B \qquad \rightarrow C + D$$

$$(7) \qquad A + B + M \rightarrow C + M$$

$$(8) \qquad A + B \qquad + C + D + E$$

$$(9) \qquad A + B \qquad \rightarrow C$$

(10)
$$A + M + C + D + M$$

The forward rate coefficient, $\mathbf{k_f}$, is input to the code as one of the following eight types

Rate Coefficient Type*

$$(1) \qquad k_{\varepsilon} = A$$

$$k_f = AT^{-1}$$

$$(3) \qquad k_{\varepsilon} = AT^{-2}$$

(4)
$$k_{\varepsilon} = AT^{-1/2}$$

(5)
$$k_f = A \exp(B/RT)$$

(6)
$$k_f = AT^{-1} \exp(B/RT)$$

(7)
$$k_f = AT^{-3/2}$$

(8)
$$k_f = AT^N \exp(B/RT)$$

^{*} Rate coefficient data for typical rocket nozzle reactions may be found, e.g., in Ref. 15.

Jensen, D.E. and Jones, G.A., "Gas-Phase Reaction Rate Coefficients for Rocketry Applications," Rocket Propulsion Establishment Technical Report No. 71/9, October 1971.

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The equilibrium constant, $\mathbf{K}_{\mathbf{p}}$, is determined from

 $\ln K_p = -\Delta G/RT$

where the Gibbs free energy, ΔG , for individual reactions is computed from the input thermodynamic data.

APPENDIX B

SAMPLE INPUT

The following is the input data file for the standard case. The first file is the TSNIC namelist input, and the second file is the FULLNOZ input.

PDATA CPL=6.96, CPS=6.72, GAMMA=1.252, HPL=3.168, HPS=2.027, PC=1210., WHOLG=23.23, SMP=708., TGG=4169., TPM=1080.,1TDI=2, WPMGT=.005, WPMT=.5.,5, RT=.0157, THJD=9., THIW=10.5, THID=10.5, NTAPE=85 TSNIC/FN02 SAMPLE TEST CASE - N5 - 2.75 IN. MOTOR 1000 1.40 7.0 0 0 50 9000 0 0.8 .01 .0001 1.0 0.1 .64400856 E+1.18575287 E+1-.44865856E+0.36280751 E-1 .9848540E-2-.28443384E 2.54410327 E 2 .58741331E 1.13572404E 2 -.8605660761 .21500497E 1 .30567063E 1-.746409672E 2 .54321457E 2 .49483627 E 1 .23301260E-3 .39467528 E-4-.51872545E-5 -.18467323E-4.50618655 E 2.33404654 E 2 .58818265 E 1.17398375 E 1-.323042618E 0 .22313547 E-1 .795173841 E-1.79212009 E 1.50738976 E 2 .60576451 E 1.134121526E 1-.14508752E 0 .88760457 E-2 .46616242 E-1-.17005027E 1.38442271 E 2 .60311014 E 1.47049758 E 1-.94291245E 0 .49087996 E-1 .60421152 E-1-.59593534E 2.51387265 E 2 .42643469 E 1.19328092 E 1-.46138274E 0 .37083135 E-1 .91852768 E-2-.19242408E 1.52824774 E 2 . CO 1 CO 2 CO2 1 H 2 H 1 DH 1 DH 2 H2 1 H2 2 H20 1 H20 2 H20 1 1 H2 2 28 0 44 0 1.00 17.0 2.00 18.0 0. 75 0. 75 0. 75 0. 75 0. 75 0. 75 C05 139. 0 1.4 H20 H 0H 125. 5 5. 50E-1 6. 9 1. 70E-1 1. 58E-2 1. 33E-1 1. 31E-1 1. 16E-5 985 0324 600. 11. 341 . 0336 9. 507 207. 2

APPENDIX C

SAMPLE OUTPUT

The following is the output at the nozzle exit for the standard case.

1

C- 2. 2694E+05		0.0 0.0 0.0		U- 2. 2430£-05		C- 23946-05	
744 9. 0940E-01		P- 5. 1712E-01 TAMP 0.		P= 9.3149E-01 TAMP 0.		P= 5.4903E-01 TAM= 0.	
T= 7 4929E+02 P. HT= - 3265E+03 T. SURNDT= 1961E+01	MOOT - 0.	Te 7. S261E-02 P HTe S269E-03 T BURBOTe . 7803E-01	4007* 4. 4007* 4. 4007* 6. 400	T= 7. 5798£+02 P- HT= -, 5271£+03 T, BUNDOT=1765£+02	4007-0.000 MODE	T= 7. 6973E+02 PHT= 9844E+03 T/VBUTE-02	MDGT= 0. MDGT= 0. MDGT= 0. MDGT= 0. MDGT= 0.
PHIS 0. 1263E-03	X= 4318E+00 X= 8884E+01 X= 1829E+03 X= 1817E+04 X= 1817E+06 X= 1677E+06 X= 1677E+06	PHI= 1.3934E-02 H=1141E-04 SI= .4672E-01	25 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	PHI= 2. 1407E-02 H= 1137E-04 BX= . 4475E-01	X	PHI- 3.0844E-02 H 1137E-04 SB 457E-01	N= 4918E-00 N= 1859E-01 N= 1859E-02 N= 1856E-04 N= 1877E-00 N= 1079E-00
Ru- 0. R- 1. 2010E-01 DELY= 1301E+00 RHO- 1907E-03	C	R- 2. 3924E-01 DELY- 1192E-00 RHD- 1924E-03	C* 1706-00 C* 1706-00 C* 1460E-05 C* 1360E-01 C* 1360E-01 C* 1360E-01	Re 3. 9472E-01 DELY= .1173E-00 RHO1944E-03	C = 1700K-00 C = 1700K-00 C = 1400K-00 C = 1400K-01 C = 1300K-01 C = 1310K-00	R= 4.7230E-01 DELY= 1194E-00 RHD= 2010E-03	C* 35006-00 C* 17006-00 C* 14606-09 C* 13006-01 C* 13006-01 C* 13006-01
XI 7.0036+01 X 7.00481+00 MA 3736+01 PT 33366+01		1= 7.003E+00 14= .3742E+01 PT= .9402E+01	PECCIE COS PECCIE COS	1= 7.0014E+00 FA= .3724E+01 PT= .3601E+01		In 6. 9784E-00 PA 3791E-01 PT 3614E-01	00 x 00 00 00 00 00 00 00 00 00 00 00 00

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P= 5.4659E-01 TAM= 0.		P= 5.3511E-01 TMF 0.	P= 5. 2947E-01 TAM= 0.	P= 5. 2203€−01 TAME 0. 03	P= 5.2634E-0. TAM= 0.
T= 7, 6559E+02 P= 5, 4 HT= -, 5265E+03 TAN= 0 8UNDOT= , 4885E+02	0.000 0.000	HT = 7.664E+02 PHT = . 324E+03 TI SUMDIT = . 7026E+03 WD0T = 0.	T= 7, 5725E+02 P= 5, 2 HT= -, 5247E+03 TAMP SUMDOT= 0, 477E+02 MDOT= 0, 477E+02 MDOT= 0, 477E+02 MDOT= 0, 477E+02 MDOT= 0, 477E+02	T= 7, 59526+02 P HT= -, 5267E+03 T HT= -, 5267E+03 T HD0T= 0, 1245E+03 T HD0T= 0, HD0T= 0.	T= 7.5673E+02 P. HT=5273E+03 T. SUMDOT= 0. WDOT= 0.
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T= 7, 5730E+62 P= 3, 2 HT= -, 5276E+03 TAMP G SUMDOT= . 1936E+03 WDOT= 0. WDOT= 0. WDOT= 0.	0.00 BME +	2000 000 000 000 000 000 000 000 000 00	MD07 = 0. S244E+02 MV1 = S244E+02 MV1 = S244E+03 MV1 = 0. MV	2000 2000 2000 2000 2000 2000 2000
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1748E+00 1178E+03 1986E-03 1700E+00 1700E+00	1330E-01 1310E-00 1310E-00 1310E-00 1170E-00 1930E-03 1300E-03 1140E-03	13300E-01 1310E-00 1310E-00 1168E-00 1929E-03 1700E-00 1160E-04 13300E-00	20-10-10-10-10-10-10-10-10-10-10-10-10-10	3190E-01 1979E-02 1700E-00 1700E-00 1160E-04 1300E-01
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1142E+04 4704E+01	X= .4518E+00	BBB6E-01	13296-03	13696-04	18176+00	16996+00	1076E+00	1.8632E-01 1143E+04 6709E+01
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MA 3739E+01	8	203	=	8	2	0	2	X= 6. 8554E+00 HA= .3740E+01 PT= .5392E+01
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17

MEDARY LAYER NOT COMPUTED

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	X- 152	E-03	POOT-		
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DOMESTICAN VELOCITY 1. 671E+05 1. 456E+05					
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1 1905+00 1					

REVNOLDS NO. = 1.843E+21 Y2= 6.253E-01 R2= 8.247E-01	REVNOLDS NO. = 1. 837E+21 Y2= 9. 443E-01 R2= 9. 432E-01	NO. = 1. 828E+21 YZ= 1. 062E+00 RZ= 1. 060E+00	REYNOLDS NO. = 1. 821E+21 VZ= 1. 179E+00 RZ= 1. 177E+00	MEYNOLDS NO. = 1.802E+21 Y2= 1.296E+00 R2= 1.273E+00	REYNOLDS NO. = 1. 783E+21 Y2= 1. 413E+00 R2= 1. 408E+00
		REVNOLDS NO.			
	2 1 2 3 1 1 5 1 5 1 5 1 5 1 5 1 5 1 5 1 5 1 5				MOPERTIES 7- 7. 537E-02 74ASE PROPERTI 1.049 1.040 1.041 1.917 1.917 1.917 1.917 1.917 1.917 1.917 1.917 1.917 1.917 1.917 1.917 1.917 1.917 1.917

REVNOLDS NO. = 1. 5375+21 YZ* 1. 513E+00	REYNOLDS NO. = 4. 6666-20 V2= 1. 5456-400 R2= 1. 5366-400	REVIDLUS NO. = 1. 471E+21 V2= 1. 640E+00	REVNOLDS NO. = 1. 4926+21 V2= 1. 7516+00 R2= 1. 7426+00	REYNOLDS ND. = 0. Y2= 0. R2= 0.
	U= 2.267E+05 T= 7.50E+02 DENBITY= 1.939E-04	U= 2.261E+03 T= 7.496E+02 DENBITY= 1.95E-04	U= 2.260E+03 T= 7.481E+02 DEWBITY= 1.935E-04	DOMESTICAL MASS PROFERTIES PARTICLE GROUP 1 2 DOMESTREAM VELOCITY 0 0